Re-engineering a nanodosimetry Monte Carlo code into Geant4: software design and first results

E. Gargioni, V. Grichine and M. G. Pia

***Abstract*—A set of physics models for nanodosimetry simulation is being re-engineered for use in Geant4-based simulations. This extension of Geant4 capabilities is part of a larger scale R&D project for multi-scale simulation involving adaptable, co-working condensed and discrete transport schemes. The project in progress reengineers the physics modeling capabilities associated with an existing FORTRAN track-structure code for nanodosimetry into a software design suitable to collaborate with an object oriented simulation kernel. The first experience and results of the ongoing re-engineering process are presented.**

I. Introduction

METHODS to model hard interactions of particles with matter constituents by means of an appropriate binary theory are well established: in this approach collisions are treated as binary processes, that is, either the target electrons are treated as free and at rest, or the influence of binding is accounted for only in an approximated way.

General-purpose Monte Carlo codes, like EGS [1], [2], [3], FLUKA [4], [5], Geant4 and MCNP [8], [9], [10], operate in this context. Their calculations of energy deposit distributions are based on condensed-random-walk schemes of particle transport; this approach is adequate as long as the discrete energy loss events treated are of magnitudes larger than electronic binding energies.

Various specialized Monte Carlo codes, usually known as "track structure codes", have been developed for microdosimetry and nanodosimetry calculations. They handle particle interactions with matter as discrete processes: all collisions are explicitly simulated as single-scattering interactions. This approach is suitable to studies where the precise structure of the energy deposit and of the secondary particle production associated with a track is essential; nevertheless, the detailed treatment of collisions down to very low energy results in a high computational demand.

There is increasing evidence that the pattern of radiation interaction on the nanometer level is critical for the biological effects of ionizing radiation; in addition, radiation effects at the nano-scale are important for the protection of electronic devices operating in various radiation environments.

In realistic use cases such small-scale systems are often embedded in larger scale ones: for instance, a component may operate within a HEP experiment or on a satellite in space, cellular and sub-cellular aggregates in real biological systems exist in complex body structures etc.

So far, simulation based on condensed-random-walk schemes and track structure generation have been treated as distinct computational domains. The separation of the two simulation domains is due to the conceptual and technical difficulty of handling the two schemes in the same simulation environment. Achieving a conceptual approach and an architectural design where the two schemes can co-work would represent a significant progress in Monte Carlo simulation.

Recently, a set of specialized processes for track structure simulation in liquid water has been designed and implemented in Geant4 [11]; like their equivalent in dedicated Monte Carlo codes, they operate in the régime of discrete interactions only. As a further step to provide the experimental community with tools for Geant4-based simulations at the nano-scale, the physics capabilities of a Monte Carlo code for nanodosimetry simulation [12] are being re-engineered for use with Geant4 kernel. This extension of Geant4 capabilities is part of a larger scale R&D project for multi-scale simulation, which investigates the concept of adaptable, co-working condensed and discrete transport schemes [17], [18].

II. Nanodosimetric distributions

Nanodosimetric quantities, like size distributions of clustered ionization, are important in understanding the radiation-induced damage in biological targets of nanometric size (such as DNA segments) [13]. These quantities, however, are not directly measurable in biological targets and their actual knowledge is mostly based on theoretical models. A practice to overcome this problem is to measure cluster-size distributions using a nanodosimeter, which consists basically of a gas-filled counter operating at low pressure.

A typical nanodosimeter, as developed in several institutions in the past few years [14], [15], [16], consists of a low-pressure interaction chamber, an electrode system to extract ions or low-energy electrons from the interaction chamber, an evacuated drift column which includes at its end a single-particle counter, and a primary-particle detector. When charged particles enter the interaction chamber, they penetrate through or pass aside a wall-less target volume of definite shape and size, and finally reach a trigger detector at the opposite end of the chamber. Ions or low energy electrons produced within the target volume are extracted from the interaction chamber and guided into an evacuated drift chamber where they are detected by a single-particle counter. If such measurements are performed for a large number of primary particles of radiation quality Q, the

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Elisabetta Gargioni is with University Medical Center Hamburg-Eppendorf, Germany.

Vladimir Grichine is with Lebedev Institute, Moscow, Russia and CERN, Geneva, Switzerland.

Maria Grazia Pia is with INFN Sezione di Genova, Genova, Italy.

final result is the probability distribution $P_n(Q)$ of ionization cluster size n.

These nanodosimeters were developed aided by the important contribution of particle-track Monte Carlo simulations. These simulations require an accurate, complete and consistent set of scattering cross sections in the gas of interest.

In order to take advantage of the geometrical modeling capabilities and the features for the description of larger scale environments available in multi-purpose Monte Carlo codes, it is desirable to integrate their capabilities with an appropriate particle-track code, capable of accurate transport of electrons with kinetic energies below 1 keV, down to the ionization threshold.

III. Reengineering process

The project in progress aims at reengineering the physics modeling capabilities of a track-structure code developed in the past years for nanodosimetry applications [12] into a set of simulation tools compatible with Geant4 kernel. The corresponding software process is based on the Unified Process [19]: it adopts an iterative and incremental life-cycle, providing concrete deliverables at each iteration.

The original "track structure" code was developed according to a procedural programming paradigm and is written in FORTRAN. The availability of its functionality for operation in an open source, general purpose simulation environment would provide experimentalists more powerful modeling capabilities for nanodosimetric studies than the original code: researchers would be able to exploit the rich functionality of other Geant4 domains, like geometry, navigation, visualization and other features, along with the specialized physics available in the original standalone FORTRAN code.

Once reengineered for use compatible with Geant4 kernel, the functionality corresponding to "track structure" simulation, i.e. pertinent to a discrete transport scheme, would provide a valuable playground for the ongoing research on co-working condensed and discrete schemes, which is the object of the Nano5 [18] R&D process.

The introduction of equivalent physics capabilities in an object oriented simulation environment is directly based on the literature documenting the physics models implemented in the original track structure system, rather than on the FORTRAN code itself. The largely different software technology adopted by the two systems prevents the reuse of the existing procedural code: a sound solution requires rethinking the software design supporting the physics capabilities in terms of an object oriented paradigm.

Therefore the whole reengineering process is performed on the ground of the pertinent physics literature: the problem domain analysis, the software design and the implementation. This process ensures the optimization of the software quality through the adoption of established best practices, and the effective investment of the limited available resources.

The reengineering process is currently going through the inception phase. Requirements are captured from the pertinent literature and analyzed; their impact on Geant4 simulation kernel is evaluated in depth. At this stage the analysis and design process explores the capability of policy-based design [20] of supporting the physics functionality of a large scale track structure code in an object oriented environment.

The agility of the design, discussed in [21], facilitates testing physics functionality thoroughly along with the implementation process: the test process can easily encompass both the verification of the correctness of the implementation and the validation against experimental data (if available) at the level of unit testing.

IV. First results: electron impact ionization

Ionization produced by slow (kinetic energy smaller than few keV) electrons is one of the main processes which should be simulated in nanodosimetry. The mean free path of electrons due to the ionization process is defined by the total ionization cross section. Here we show some preliminary results concerning the implementation of the Binary Encounter Bethe (BEB) model for the total ionization cross section of slow electrons with atoms and molecules. The model has been implemented in a policy-based class design similar to the approach adopted in [21] to model photon interactions.

A. Binary encounter Bethe model

According to the binary encounter Bethe model [22], the total ionization cross section of slow electrons for an atomic shell, i, with binding energy B_i reads:

$$\sigma_i(t) = \frac{S_i}{t+u+1} \times \left\{ \frac{Q_i}{2}\left(1-\frac{1}{t^2}\right)\ln t + (2-Q_i)\left[\left(1-\frac{1}{t}\right) - \frac{\ln t}{t+1}\right]\right\},$$

$$t = \frac{T}{B_i}, \quad u = \frac{U_i}{B_i},$$

where $S_i = 4\pi a_o^2 N_i (R/B_i)^2$, R is the Rydberg energy (13.61 eV), a_o is the Bohr radius (5.29×10^{-11} cm) and N_i is the number of bound electrons in the i-shell. T is the kinetic energy of the incident electron, and U_i is the average kinetic energy of the i-shell electrons. The Q_i value relates to the atomic oscillator strength distribution, df/dw:

$$Q_i = \frac{2}{N_i}\int_0^\infty \frac{1}{w+1}\frac{df}{dw}dw, \quad w = \frac{W}{B_i},$$

where W is the kinetic energy of the ejected (ionization) electron.

In the cases, when the distribution df/dw is unknown, one can set $Q_i = 1$ [23]. Then equation (1) can be simplified:

$$\sigma_i(t) = \frac{S_i}{t+u+1}\left\{\frac{\ln t}{2}\left(1-\frac{1}{t^2}\right) + 1 - \frac{1}{t} - \frac{\ln t}{t+1}\right\}. \quad (1)$$

The total ionization cross section is defined by the summation of equation (1) over all involved atomic shells. The number of the shells, as well as the shell parameters, can be either parametrized for molecules [24], or derived from atomic databases [22].

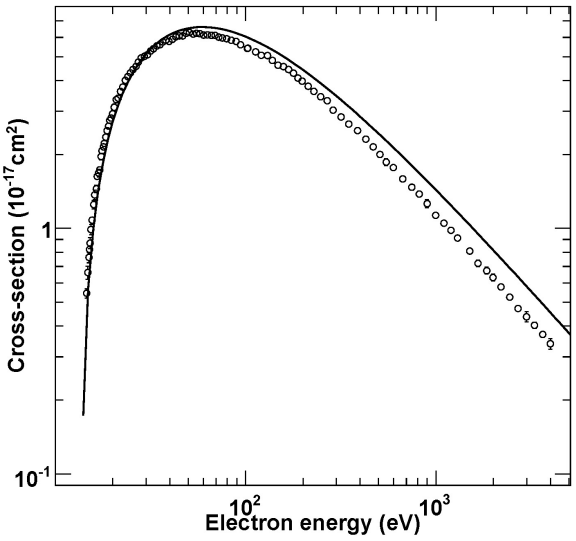

Fig. 1. Total cross section for ionization of atomic hydrogen by low energy electrons. Experimental data (open circles) are from [25], the solid line is our simulation according to equation (1).

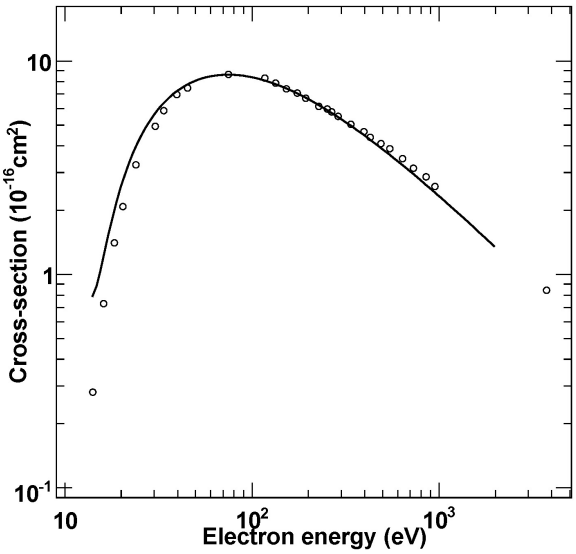

Fig. 2. Total cross section for ionization of C_3H_8 by low energy electrons. Experimental data (open circles) are from [26], the solid line is our simulation according to equation (1). The propane molecular parameters used in the simulation were parameterized in [24].

B. Comparison of simulation with experimental data

The total ionization cross section simulated according to the summation of equation (1) over all involved atomic shells was compared with experimental data for hydrogen and propane. Fig. 1 shows the energy dependence of the ionization cross section of electrons on atomic hydrogen. Experimental data (open circles) are from [25], the solid line is our simulation according to equation (1).

Fig. 2 shows the energy dependence of the electron impact ionization cross section for propane. Experimental data (open circles) are from [26], the solid line is our simulation according to equation (1). The propane molecular parameters used in the simulation were parameterized in [24].

These preliminary comparisons show satisfactory agreement of our simulation with experimental data.

A significant metric in the reengineering process is the time investment for the achievement of these results: it amounted to a few days' work, including the study of the pertinent literature, the implementation of the physics model, the verification of the software and the validation against experimental data.

V. Conclusion and Outlook

A process is in progress to reengineer the physics capabilities of an existing software system for nanodosimetry simulation in a software environment compatible with Geant4 kernel; as a further step, the seamless transition of transport schemes between nanodosimetric and conventional dosimetry simulation will be object of investigation.

The first results of the reengineering process are encouraging: they document the feasibility of implementing the cross section model in a policy class, the achievement of satisfactory physics accuracy and a preliminary estimate of the expected development effort.

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